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Correcting heat storage in a calorimetric chamber by a two-compartment-model[1]

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Abstract

Direct calorimetry is used for investigating combustion energy of fuels, thermic properties of materials and metabolic processes. Its results, however, may be influenced by the dynamic properties of the equipment, if they are not much faster than those of the subject. When performing direct calorimetry at living beings, the dynamic properties of the system chamber–interior–subject must be taken into account. A simple model is known to correct for the dilution of metabolic gases in the chamber. Heat, however, is not simply diluted; it is stored in the chamber's interior and the subject's body too. A two-compartment-model was shown to correct heat storage effects in a furnished human calorimetric chamber. A method was established to estimate proper model parameter from alcohol combustion as calibration experiments. Heat storage resulted in $7.8 + 1.1\%$ of all heat measured after extinguishing the flame. The 'wake period' lasted more than 3 h. Using the two-compartment-model this was overcorrected to $-1.6 + 1.9\%$ with the 'wake period' being less than 15 min. Humans or animals in the chamber would change the model parameter dramatically due to their large heat capacity. The corresponding parameters could not be derived from only a few calibration experiments; more work needs to be done in the future. © 1997 Elsevier Science B.V.

Keywords: Direct calorimetry; Dynamic parameter; Heat dilution; Two-compartment-model

1. Introduction

The methods of direct and indirect calorimetry have long been used to estimate heat loss (HL) and energy expenditure (EE) of both human subjects and animals [1–4]. The most recent survey on methods to assess HL and EE [5] showed, that direct calorimeters are rarely used to investigate energy metabolism, especially by nutritionists. There are other groups [6] using a direct calorimeter to estimate heat production of insects. But overall, most groups use indirect calorimeters that provide not only values for EE, but information on the substrate oxidation rates as well. There are well-established methods to deal with gas dilution in the chamber [7,8]. These methods apply to direct calorimetry too, but due to heat not stopping at the surface of calorimeter and furniture they are not sufficient to model and compensate heat storage in the chamber. Simultaneous direct and indirect calorimetry however could be used to gather information on the

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time-course of protein oxidation rate in subjects (Frenz and Rumpler, submitted to Br. J. Nutr.). This information is usually assessed within periods of some 8 h to a full day, whereas the periods of interest for nutritionists are of the order of a few minutes. For this purpose heat storage in calorimetric chambers has to be compensated.

Direct calorimeters may even react faster than indirect ones and can serve as useful tools for investigating heat transport and storage effects in the subject's body. While entering or exiting the chamber, subjects may transport different amount of heat that has to taken into account. This could be done by strong limitations in the experimental schedule to avoid these differences or by compensating for them.

2. Methods

2.1. Theory

There are methods to take into account the dilution of metabolic gases in the calorimetric chamber. Usually the chamber is counted as one large storage compartment, where any gas change is assumed to be immediately mixed and then slowly removed by the flow of air. This behaviour can be described by the following partial differential equation [9]:

$$\frac{\mathrm{d}C_1(t)}{\mathrm{d}t} = \frac{-F}{V} C_1(t) = \frac{-1}{\tau_1} C_1(t) \qquad (1)$$

where,

$C_1(t)$	actual concentration of O_2 or CO_2 in the chamber
F	flowrate of air through the chamber
V	effective volume of the chamber
$\tau_1 = V/F$	time constant of the system

Thus, the product of the 1st derivative of $C(t)\,C'(t) = \mathrm{d}C(t)/\mathrm{d}t$ and the effective chamber volume is equal to the actual gas flow into, or out of the chamber. Because all these concentrations are counted as change relative to the concentration at time $t = 0$, the resulting gas flow, which is the product of air flow rate and gas concentration, has to be looked upon as a corrective term to the basal flow . The same can be done for the components of HL, which are measured by water vapour flow and temperature of the chamber. But, there are more potential pools for HL in which heat can be stored. These are the chamber (the material it is made from), all the furniture usually inside it and the subject itself. To model this situation, a simple one-compartment model is insufficient and at least a two-compartment model has to be used instead, namely:

$$\frac{\mathrm{d}C_1(t)}{\mathrm{d}t} = -\frac{1}{\tau_1}\left[C_2(t_0)e^{-\frac{t-t_0}{\tau_2}}\right] - \frac{1}{\tau_1}C_1(t)d \qquad (2)$$

where $C_2(t)$ is the concentration on the 1st compartment (inside chamber walls, furniture, etc.), whereas all measurements are done at the (now) 2nd compartment – the entire chamber.

Unfortunately, there is no simple solution for this equation as for Eq. (1). One has to solve it instead, assuming that $C_1(t_0) = 0$:

$$C_1(t) = C_2(t_0)\frac{\tau_2}{\tau_2 - \tau_1}\left[e^{-\frac{t-t_0}{\tau_2}} - e^{-\frac{t-t_0}{\tau_1}}\right] \qquad (3)$$

This is a double exponential function, which starts at 0, reaches a peak at $t_m = -\ln(\tau_1/\tau_2)/(1/\tau_1 - 1/\tau_2)$ and returns to 0 similar to a normal exponential function with a negative time constant. A very similar curve is obtained as the 'wake' of HL if one ignites an alcohol burner in the chamber, lets it run for some time and then extinguishes it (Fig. 1, enlarged in Fig. 2). Changes in heat storage are driven by a temperature change $T' = \mathrm{d}T/\mathrm{d}t$ and are proportional to this. So, $C_2(t_0)$ is somehow mapped to $T'(t_0)$.

2.2. The combined direct and indirect calorimetric chamber in Beltsville

This chamber is one of the very few remaining combined direct and indirect calorimeters. It is a 20.4 m^3 chamber, designed to house human volunteers comfortably for 24 h periods or longer, allowing the measurement of the subject's HL and EE [4]. The chamber is furnished with a futon bed, a desk and chair, a wash basin, a portable toilet and an exercise bike. The subjects can control a TV, VCR and stereo through one of the chambers' windows. The audio signal is provided by small self-amplifying speakers inside the chamber. Gas concentrations in the chamber

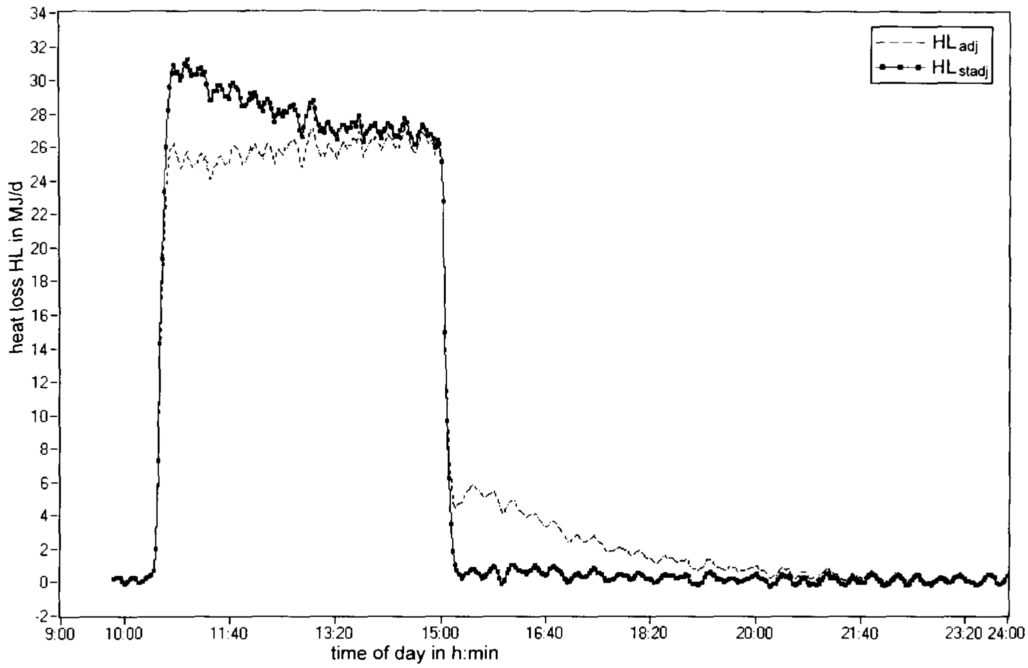

Fig. 1. Effect of heat storage compensation on heat loss in an alcohol combustion experiment: comparison of uncompensated data (HL_{adj}) and compensated data (HL_{stadj}).

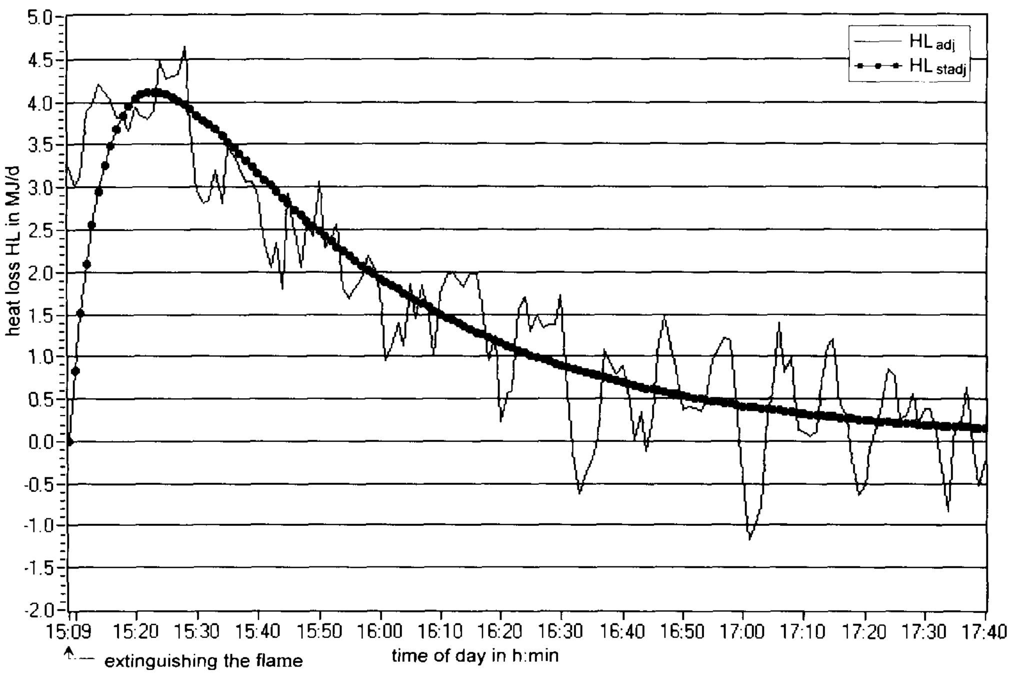

Fig. 2. Data of the alcohol combustion experiment shown in Fig. 1 after extinguishing the flame: HL_{adj} and best fit for a double exponential function.

are measured by a multiple gas analyzer/mass spectrometer MGA 1200 (Perkin-Elmer, Pomona, CA). Heat flow through the chamber walls is estimated by a gradient layer, whereas heat transfer by air and evaporative heat losses are monitored by airflow and humidity measurements. All entering electrical energy is monitored. All measurements are controlled by a personal computer program; the raw data are stored for later evaluation.

2.3. *Programming and calculations*

The data acquisition system provides data for each experiment in an ASCII-File. It contains all data of direct and indirect calorimetry, acquired every two minutes as average values. All calculations on the data presented in this paper are done with a program created with LabView™ (National Instruments, Austin, TX), a graphical programming system for data acquisition, visualization and analysis. The program is structured into more than 70 subroutines, organized in 7 hierarchical levels. Some of the most important steps are:

- The data file is read, the data are transferred into the native LabView format. They are filtered by a lowpass Bessel filter of 1st order with the highest possible cut-off frequency to reduce noise. A raw compensation of gas and heat storage is performed to enable the user to select a period of interest. If this period contains calibration data (Fig. 2) the parameter for the model can be estimated by a subroutine:
  - The last 10% of the data are used to perform a logarithmic fit and estimate the time constant t and amplitude A of an exponential function. Also time (t_m) and amplitude of the maximum (y_m) are detected by smoothing the data around its maximum to a quadratic function. An empirical formula is used to estimate τ_1 and filter the data with a Bessel filter of 10th order and a cut-off frequency of $3\pi/\tau_1$.τ_1 is re-estimated from the filtered data.
  - Utilizing the mathematical properties of the assumed function, τ_2 is detected from τ_m by an iterative process. The double exponential function is calculated with τ_1, τ_2 and an amplitude $A = 1$. Its results, as well as the original data are integrated. The quotient of both integrals accounts for A. The sum of the squared differences between the fitted signal and the raw data is calculated as a measure of quality of fitting.
  - τ_1 is varied in another iterative process in an attempt to improve the fitting by decreasing the sum of squared differences between data and fit. This is repeated until its variation becomes marginal ($\Delta\tau_1 < 1$s).
  - Finally, the results of fitting and the raw data are shown in a graph (Fig. 2) and the double exponential fit parameter are saved in a parameter file.
- The compensation of gas dilution in the chamber is performed according to Eq. (1), resulting in the adjusted energy expenditure EE_{adj}. The same is done for heat and water storage in the chamber's air, resulting in the adjusted heat loss HL_{adj}.
- The values of $T' = dT/dt$ are multiplied by the quotient A/T'^{-2}, and this value is used as the new (time dependent) amplitude. This parameter together with the time constants are then used to calculate the influence of every signal change to its successors with the help of the double exponential function. All these influences are balanced for every period and subtracted from HL_{adj}, resulting in HL_{stadj}.

2.4. *Conditions for parameter determination*

Calibration or standard data are needed to determine the model parameters. This can easily be achieved in alcohol combustion experiments by extinguishing the flame after some time. The resulting HL_{adj} should ideally fall back to zero. The real HL_{adj} does not behave in this way because of heat storage effects (Fig. 1). However, appropriate model parameters should compensate these heat storage effects. Unfortunately, the model parameters for a chamber

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[2]The model parameter was estimated for a just extinguished alcohol lamp. The amplitude A was proportional to the corresponding temperature decrease, which was the most negative $T'(T'^{-})$. This proportionality is removed by calculating the quotient A/T'^{-}.

with subject are not so easy to determine. The subject's metabolism changes due to diverse reasons with diverse rhythms, ranging from a few seconds (locomotor activity) to several hours (thermic effect of food). One cannot expect to obtain a constant value for an appropriate time to fit the data to the double exponential function. Even while sleeping there are some unconscious movements that raise EE and HL temporarily or, virtually, by uncovering of heated parts of the subject's body or the futon bed. These raises would influence the estimation of model parameters. Hence, the detection algorithm cannot be applied to normal measurements on humans. One possible way might be to allow people to enter the chamber after having a small meal. They should try to maintain a moderately high level of activity without sweating for ~3 h. This should introduce a high heat content not only into their body but into the chamber's interior as well. Then, they should be allowed to rest, to sleep if possible, and to maintain themselves in that state for at least 5 h. In this case, one should expect a relatively large decrease in overall HL, and relatively constant levels of HL before and after this decrease. Minor unconscious movements should not count as important compared with the high decrease of HL while changing from moderate activity to rest. These may even be eliminated by an iterative process, using a first estimation of the model parameter.

2.5. *Timing*

The experiments performed for an estimation of the influence of heat storage in the chamber's interior were divided into two phases. The active phase started with someone entering the chamber or igniting the alcohol flame and finished on his leaving the chamber or extinguishing the flame. The second phase began immediately after the active phase ended, and lasted as long as the active phase. This has been called the 'wake phase'. The time of entering/leaving or igniting/extinguishing was not recorded relative to the computer timer, hence a routine to detect these times was established. The beginning of the active phase was determined as the first time when HL'_{adj} was above a defined threshold. Its end was, correspondingly, the last time when HL'_{adj} was below that threshold. The threshold was determined to be absolutely higher than the noise of HL'_{adj}.

3. Results

3.1. *Compensation of heat storage*

The heat storage compensation was checked on three different types of experiments:

- six alcohol combustion experiments
- two specially designed experiments to detect the time resolution of the methods
- six human experiments (2 × 24 h, with and without exercise (data from another study))

The time constants were estimated from the alcohol experiments. Their results varied without recognizable reason due to different positions of the alcohol combustion equipment and size and number of alcohol lamps. The time constants have been chosen to give best compensation for all alcohol experiments. The used values and the variation area were: $\tau_1 = 82$ min (57 to 116 min) and $\tau_2 = 11.6$ min (8.5 to 32 min), respectively.

Two different formulae were used in the alcohol experiments to estimate EE from gas exchange. The Weir-formula calculates EE from oxygen consumption and carbon dioxide production. A simple proportionality of the combustion energy (CE) of alcohol to the mass flow of CO_2 and O_2 out of/into the chamber (alc-formula)[3] was also used. The integral of CE in the active phase was used as standard for all other results. These relative heat losses (rHL) are easier to compare for different experiments. The results are shown in Table 1. A wake of relative heat measured after extinction of the alcohol lamp of $rHL_{adj} = 7.8 \pm 1.9\%$ of the overall combustion energy is overcompensated to $rHL_{stadj} - 1.6 \pm 1.9\%$.

Two experiments were performed to estimate the time resolution of the Beltsville chamber and to test the model and parameters, determined in alcohol combustion experiments. The subjects entered the chamber and settled down. After ~90 min, they started the first of the four repeated moderate cycling periods over 30 min with decreasing rest periods. The rest periods ranged from 120 to 5 min (Fig. 3).

[3]The Weir-formula is adapted to a food mixture. It deals with protein oxidation too. This causes some minor errors if no protein oxidation takes place.

Table 1
Comparison of some methods for estimating relative heat loss (rHL) as a quotient of heat loss by combustion energy (CE) in alcohol combustion experiments

Overall (rHL_{adj}/ (%))	Active (rHL_{adj}/ (%))	Wake w/o storage compensation (rHL_{adj}/ (%))	Wake with storage compensation (rHL_{stadj}/ (%))
104.7 ± 2.5	98.3 ± 1.0	7.78 ± 1.91	-1.59 ± 1.91

Shown are mean ± std; all results are different ($p<0.01$). The active phase is the period alcohol was actually burned; the period thereafter accounted for a wake period, being as long as the active period.

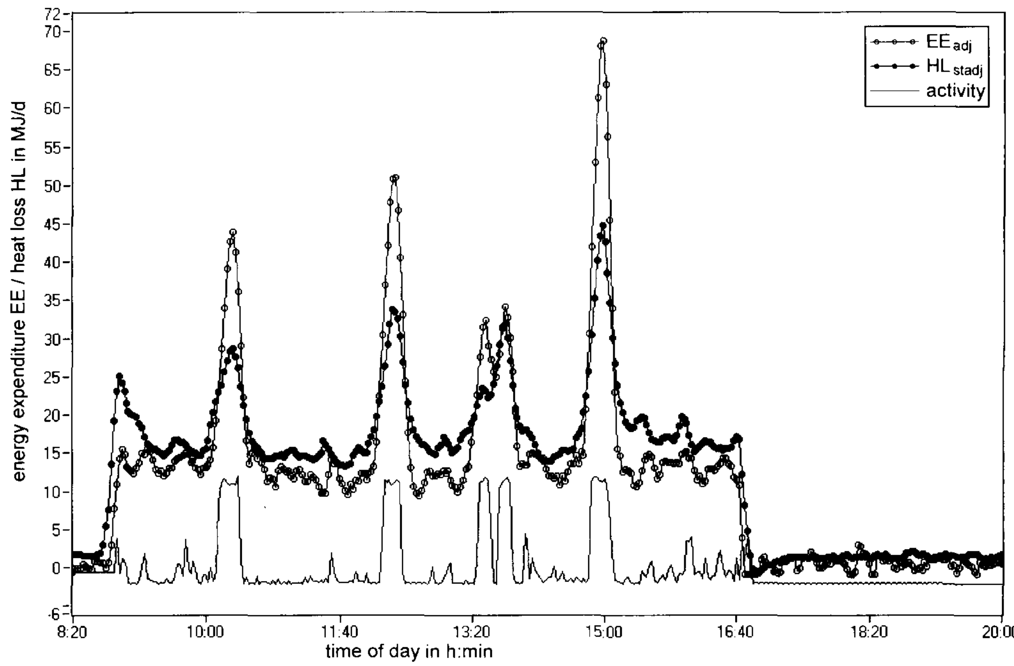

Fig. 3. Time-course of EE_{adj}, HL_{stadj} and LA in a time resolution experiment. Even resting or activity periods of just 5 min can be detected by the improved method.

Whereas peaks in locomotor activity (LA) could clearly be separated even with a rest period of only 5 min, this could not clearly be done with EE_{adj} and HL_{stadj}. The separation of EE_{adj} was much better than that of HL_{stadj}, indicating the influence of the huge heat capacity of the subject's body. To compare the results of both experiments EE_{adj} and HL_{stadj} were integrated over the active period. The integral of EE_{adj} was used as a standard. This resulted in $HL_{adj} = 92.2 \pm 1.9\%$ of EE_{adj} without compensation. After compensation, this improved to $HL_{stadj} = 98.9 \pm 0.1\%$, respectively. It is important to note, that the subjects entered and left the chamber in a rather balanced state, without carrying large amounts of heat in or out.

To test this method, some results of older studies were recalculated. In those experiments the subjects stayed twice in the chamber, ~23.5 h each time. One measurement day included moderate work on a bicycle whereas the other did not. Those measurements were not performed to be used with this method, which led to some problems while re-evaluating the data. The energy status of both the chamber and subjects at the time of entering was not very well determined[4] and the measurements were stopped

[4]Due to cleanup and preparation for the next run, the staff had to enter the chamber, thus disturbing its equilibrium. The subjects in this study were allowed to settle down in the chamber. Hence, they may or may not have had some exercise before entering.

immediately after the subject left the chamber. Thus, there were no really relevant data for storage correction to work with. Nevertheless, it introduced an average correction $\Delta HL_{adj} = 65 + 86\,kJ/d\,(0.75+1.00\,W)$, which is 0.6% of ΣHL_{adj}. On one occasion, however, there was data prior to and after the active phase and the correction resulted in $\Delta HL_{adj} = 335\,kJ/d\,(3.9\,W)$ or 2.6% of HL_{adj}. This demonstrates the need to determine this correction and to change the experimental schedule to carry out at least 10 to 15 min pre- and post-measurement.

4. Discussion

The influence of heat storage in direct calorimetry may be substantial (Fig. 1, Table 1). It can reach values up to 8% of the integral of overall HL. When huge changes in the thermic equilibrium of the system subject–interior–chamber occur, this value may be even higher. This may happen while entering or leaving the chamber, if large changes in LA occur or if subjects having a different body temperature are interchanged, as when measuring from one person to another. Interchanging subjects in a chamber without letting the system coming to some equilibrium is in fact a continued measurement. One cannot necessarily divide such continued measurements into smaller periods without taking into account the storage effects. A possible way to solve these problems is to model the influence of heat storage as a double exponential function. This model has been shown working very well on a chamber without a subject, when alcohol combustion experiments are conducted. The model should work with a subject in the chamber as well. However, this situation is difficult to calibrate. The calibration routine needs some standard values, which can easily be reached in an alcohol combustion experiment.

The routine needs more than $2^{*}\tau_1 = 164\,min$ to obtain a good estimation of the model parameter. But living subjects usually change their energy expenditure and heat loss in shorter time periods. They have a distinctive daily rhythm of EE due to food intake and locomotor activity. Subjects going to bed change their thermic resistance relative to the surrounding chamber. This would not reflect the normal and more interesting situation during the different activity and eating cycles. A special schedule for the subject's activity and sleeping pattern may overcome these problems. The model parameter, however, should be influenced by the subject's body mass due to different heat capacity. It therefore needs more effort to obtain these parameters and their dependence on the body mass of the subject.

Direct calorimetry is shown to be a very good research tool for investigating thermic response of subjects such as thermic effect of food as well as locomotor activity or thermic reactions of diseases (fever); moreover, as long as the subjects do not start to sweat the effective reaction time of a direct calorimeter may be faster than that of an indirect one.

Acknowledgements

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